Michaelis-Menten reaktionskinetik

```
> restart
```

https://en.wikipedia.org/wiki/Michaelis%E2%80%93Menten_kinetics#Derivation

Differentialligningssystemet fra WikiPedia:

$$\begin{aligned} d[S]/dt &= -k_f[E][S] + k_r[ES] \\ d[E]/dt &= -k_f[E][S] + k_r[ES] + k_{cat}[ES] \\ d[ES]/dt &= +k_f[E][S] - k_r[ES] - k_{cat}[ES] \\ d[P]/dt &= +k_{cat}[ES] \end{aligned}$$

Differentialligningssystemet opskrevet i matematisk notation:

$$\begin{aligned} S'(t) &= -k_f \cdot E(t) \cdot S(t) + k_r \cdot ES(t) \\ E'(t) &= -k_f \cdot E(t) \cdot S(t) + k_r \cdot ES(t) + k_{cat} \cdot ES(t) \\ ES'(t) &= +k_f \cdot E(t) \cdot S(t) - k_r \cdot ES(t) - k_{cat} \cdot ES(t) \\ P'(t) &= +k_{cat} \cdot ES(t) \end{aligned}$$

Differentialligningsystemet defineres i Maple.
4 differentialligninger med 4 funktioner:

```
> DL1 := S'(t) =-k_f·E(t)·S(t) +k_r·ES(t)
```

$$DL1 := \mathrm{D}(S)(t) = -k_f E(t)\, S(t) + k_r\, ES(t) \quad (1)$$

```
> DL2 := E'(t) =-k_f·E(t)·S(t) +k_r·ES(t) +k_cat·ES(t)
```

$$DL2 := \mathrm{D}(E)(t) = -k_f E(t)\, S(t) + k_r\, ES(t) + k_{cat}\, ES(t) \quad (2)$$

```
> DL3 := ES'(t) =+k_f·E(t)·S(t) -k_r·ES(t) -k_cat·ES(t)
```

$$DL3 := \mathrm{D}(ES)(t) = k_f E(t)\, S(t) - k_r\, ES(t) - k_{cat}\, ES(t) \quad (3)$$

```
> DL4 := P'(t) =+k_cat·ES(t)
```

$$DL4 := \mathrm{D}(P)(t) = k_{cat}\, ES(t) \quad (4)$$

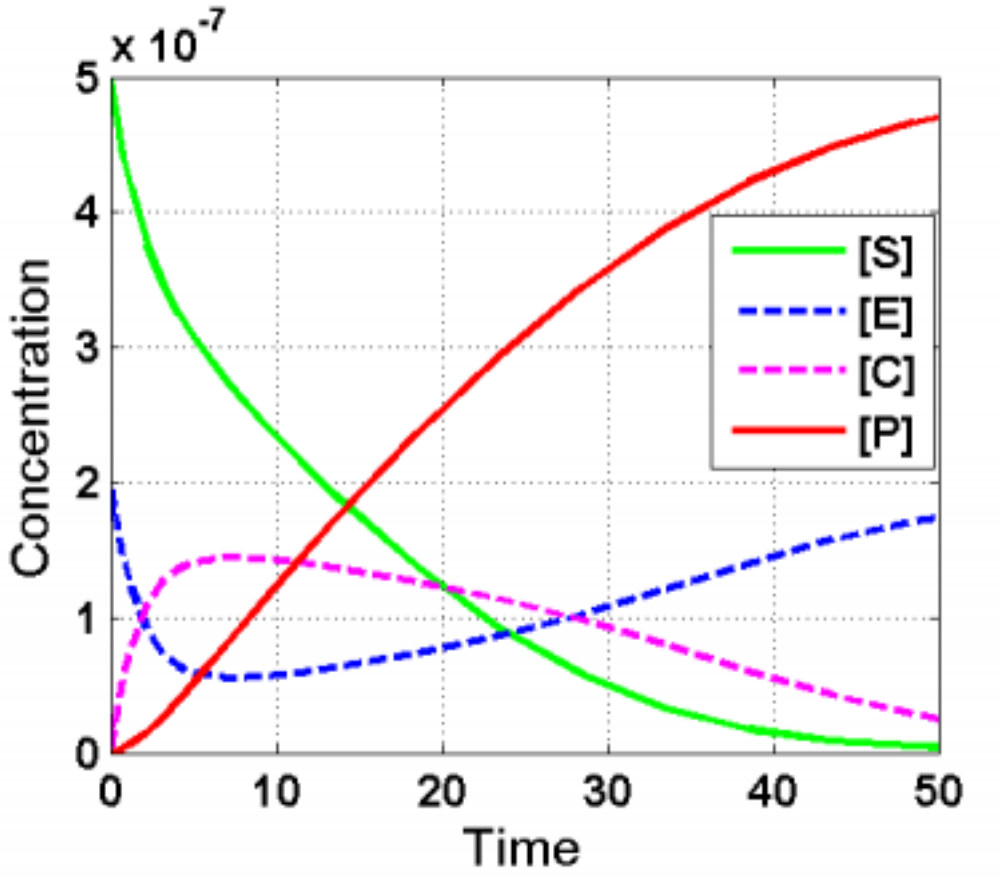
Begyndelsesbetingelser:

http://se.wtb.tue.nl/sewiki/biological_systems/de#michaelis-menten_kinetics
NB: link virker IKKE!

- $S(0) = 5e^{-7}$,
- $E(0) = 2e^{-7}$,
- $C(0) = 0$,
- $P(0) = 0$,
- $k_1 = 1e^{6}$,
- $k_2 = 1e^{-4}$,
- $k_3 = 0.1$.

Forventet graf:

http://se.wtb.tue.nl/sewiki/biological_systems/de#michaelis-menten_kinetics
NB: link virker IKKE!



> $k_f := 1 \cdot 10^{6}; k_r := 1 \cdot 10^{-4}; k_{cat} := 0.1$

$$k_f := 1000000$$

$$k_r := \frac{1}{10000}$$

$$k_{cat} := 0.1 \quad \textbf{(5)}$$

Numerisk løsning af differentialligningssystemet:

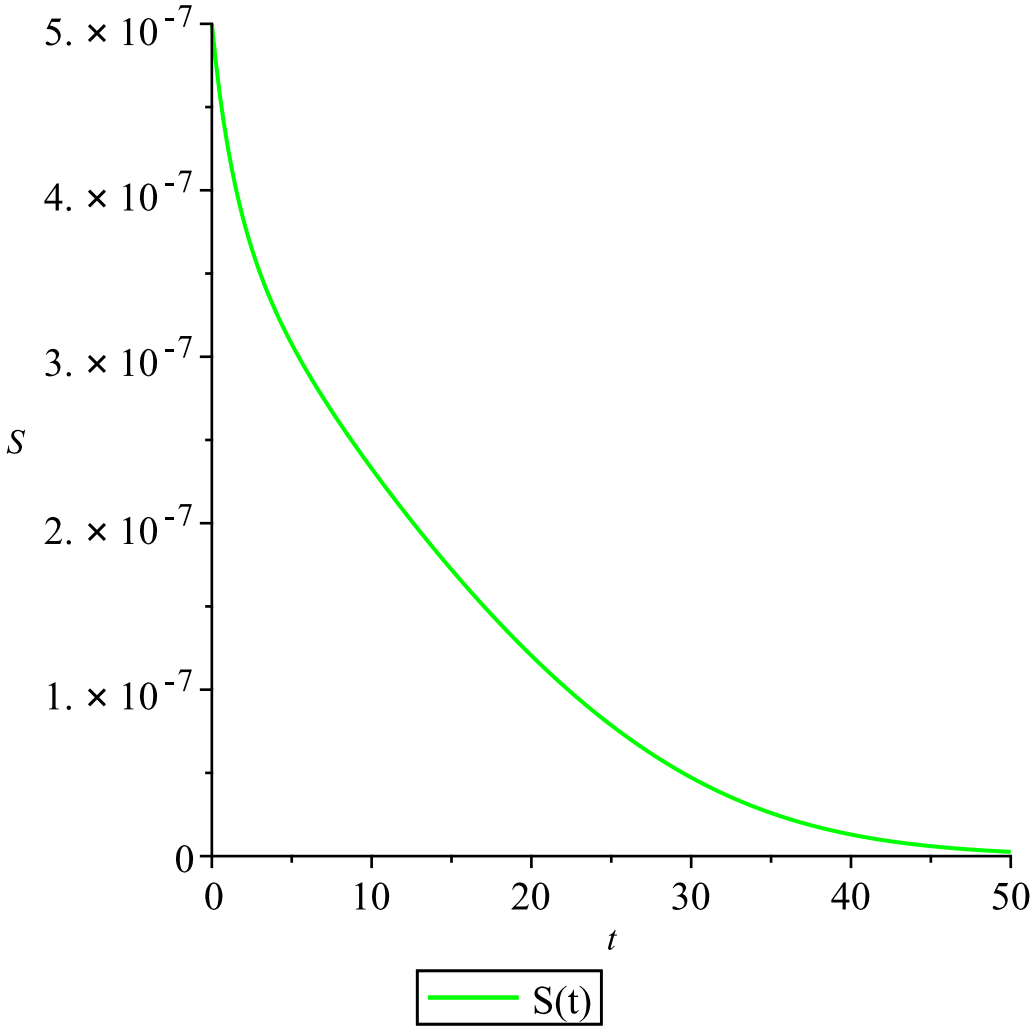
https://en.wikipedia.org/wiki/Numerical_methods_for_ordinary_differential_equations

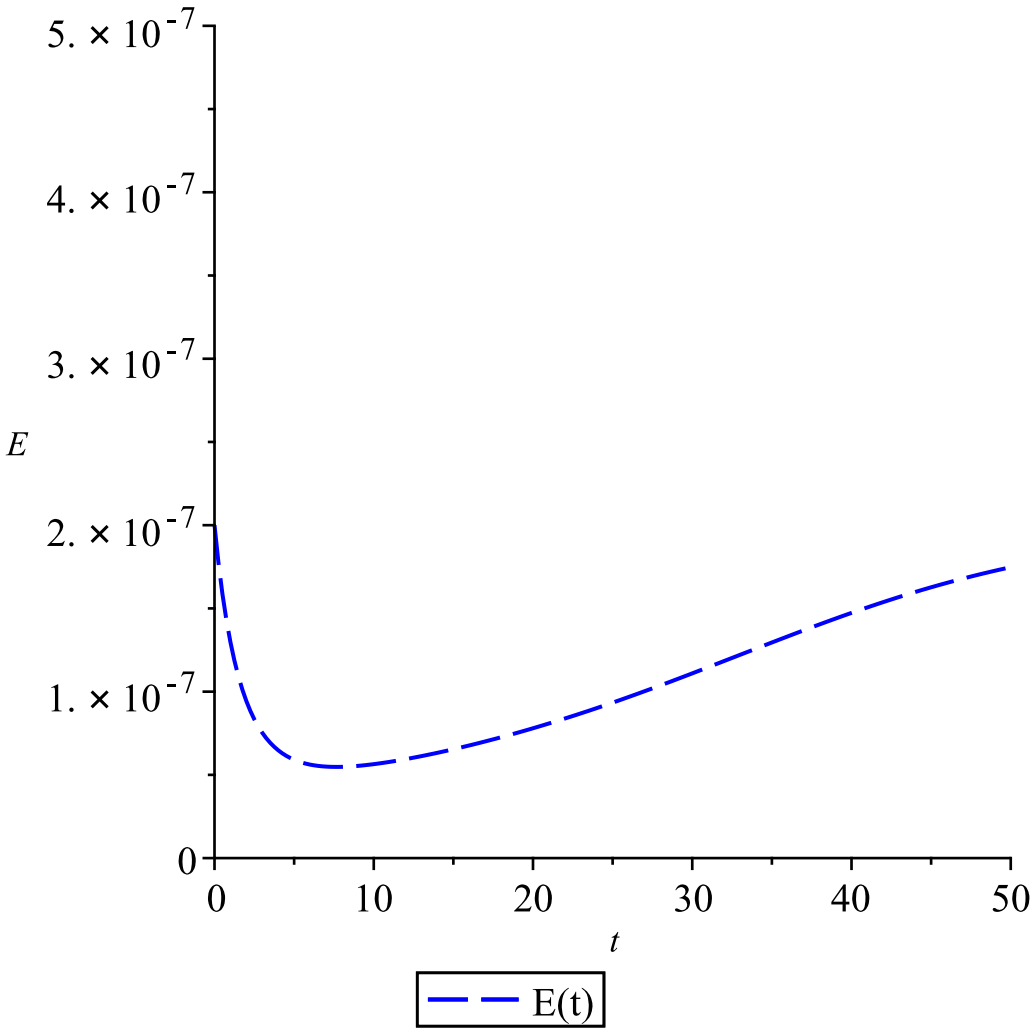
https://en.wikipedia.org/wiki/Runge%E2%80%93Kutta_methods

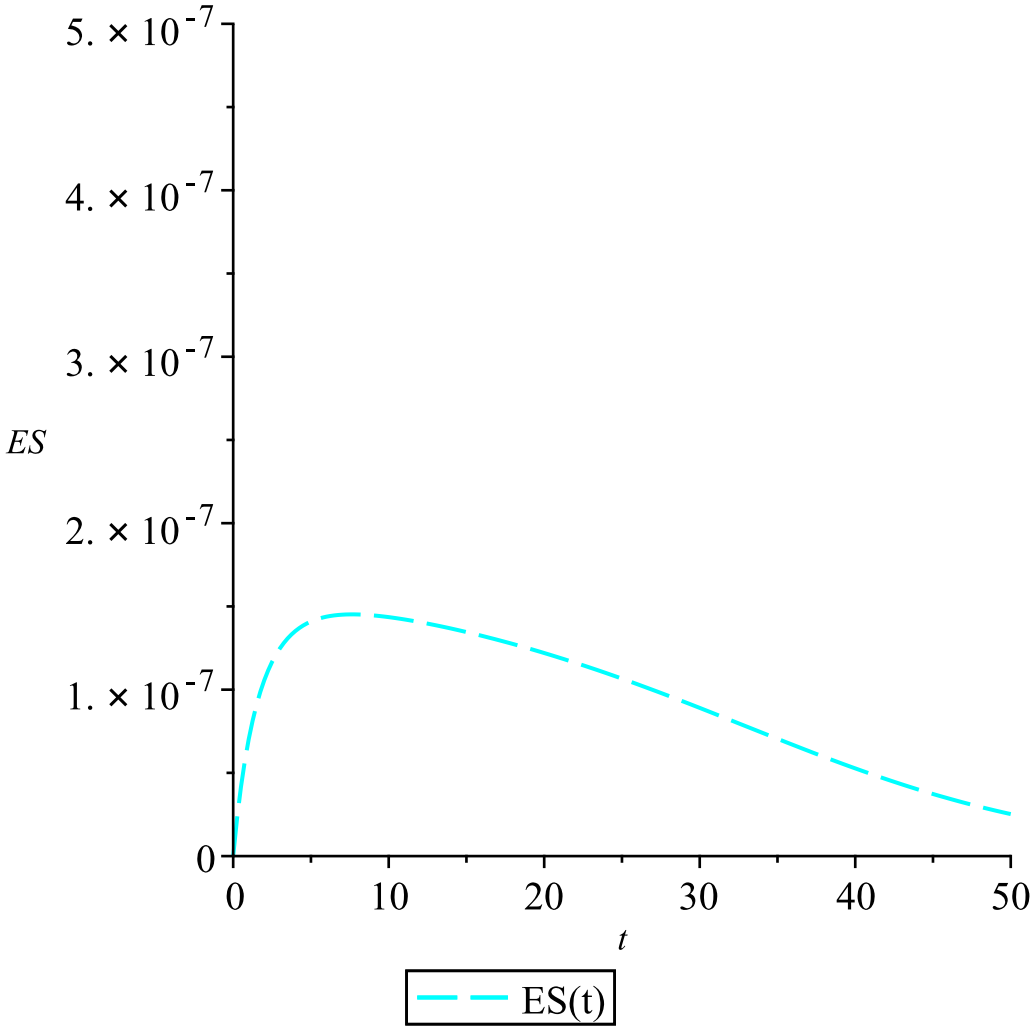
https://en.wikipedia.org/wiki/Runge%E2%80%93Kutta%E2%80%93Fehlberg_method

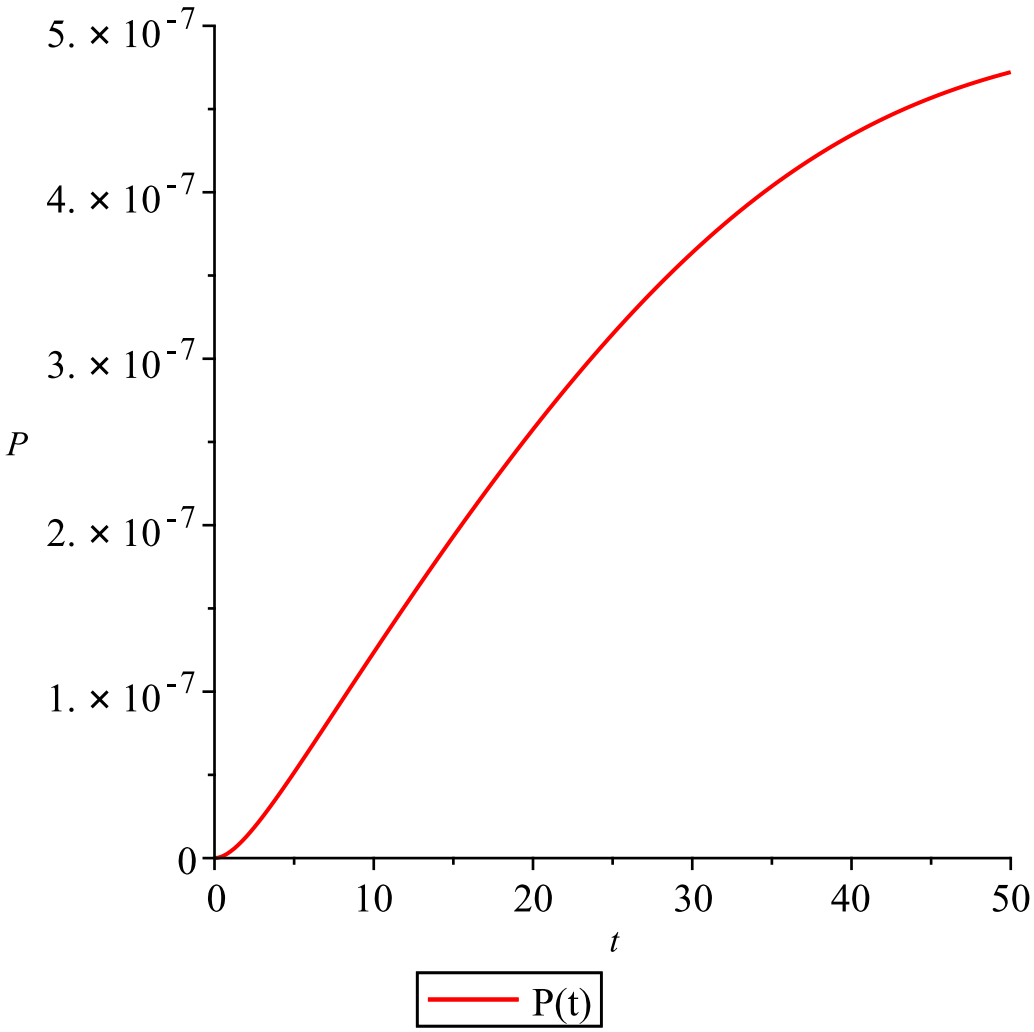
Differentialligningssystemet løses numerisk (tilnærmet), da det ikke kan løses eksakt:

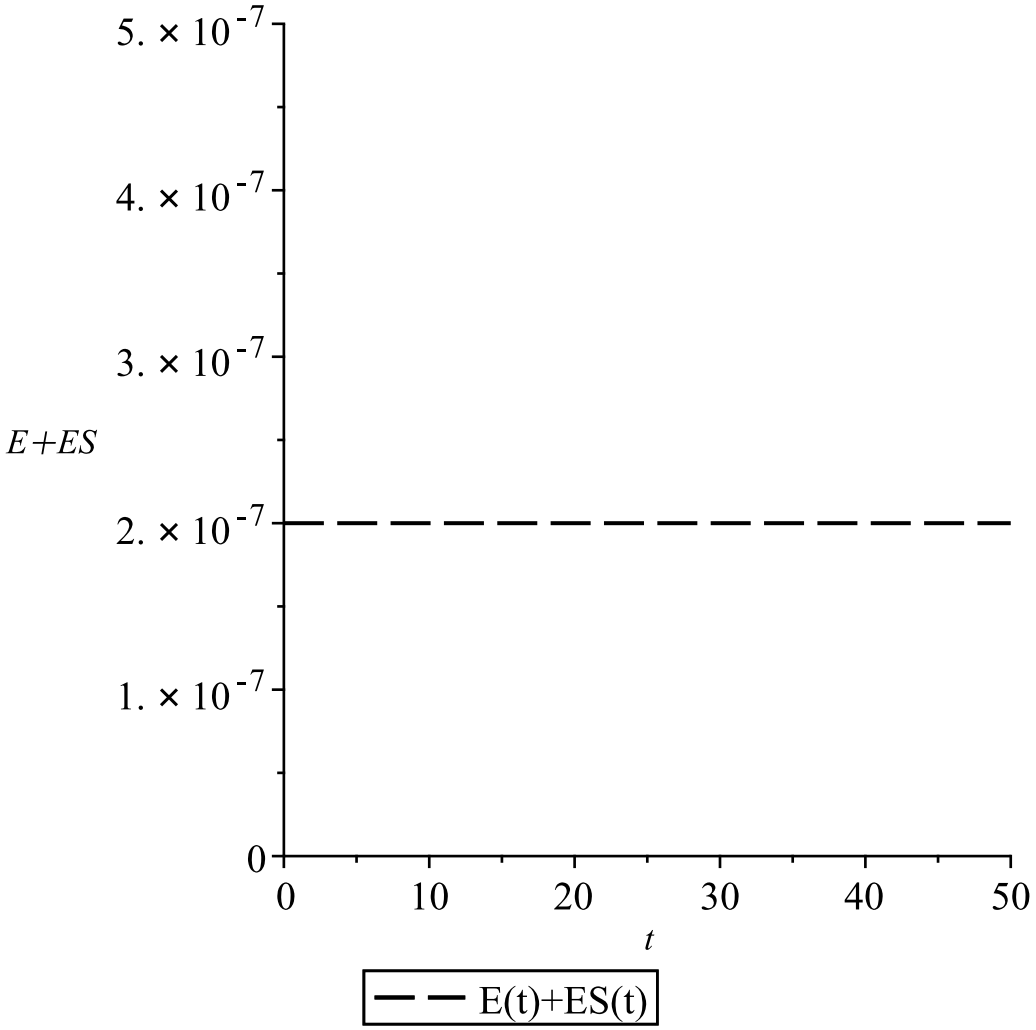
```
> løsning := dsolve({DL1, DL2, DL3, DL4, S(0) = 5·10^-7, E(0) = 2·10^-7, ES(0) = 0, P(0)
      = 0}, numeric, method = rkf45, abserr = 10^-10) :
> with(plots) :
> odeplot(løsning, [t, S(t)], t = 0..50, color = green, legend = "S(t)") : plotS := %:
      display(plotS, view = [0..50, 0..5·10^-7]);
  odeplot(løsning, [t, E(t)], t = 0..50, color = blue, linestyle = dash, legend = "E(t)") : plotE :=
      %: display(plotE, view = [0..50, 0..5·10^-7]);
  odeplot(løsning, [t, ES(t)], t = 0..50, color = cyan, linestyle = dash, legend = "ES(t)") :
      plotES := %: display(plotES, view = [0..50, 0..5·10^-7]);
  odeplot(løsning, [t, P(t)], t = 0..50, color = red, legend = "P(t)") : plotP := %:
      display(plotP, view = [0..50, 0..5·10^-7]);
  odeplot(løsning, [t, E(t) + ES(t)], t = 0..50, color = black, linestyle = dash, legend
      = "E(t)+ES(t)") : plotEES := %: display(plotEES, view = [0..50, 0..5·10^-7]);
```



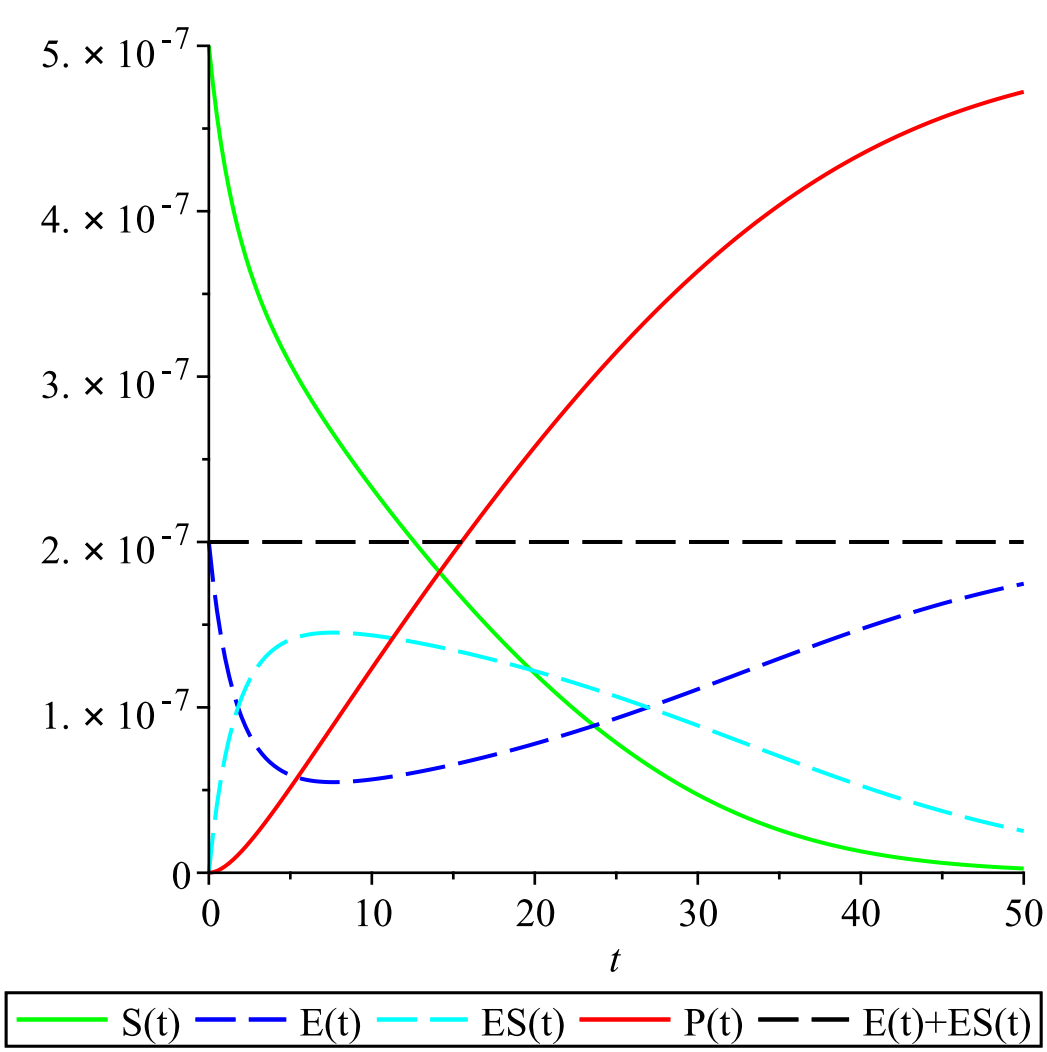

5. × 10^-7
4. × 10^-7
3. × 10^-7
E
2. × 10^-7
1. × 10^-7
0
0
10
20
30
40
50
t
E(t)


5. × 10^-7
4. × 10^-7
3. × 10^-7
ES
2. × 10^-7
1. × 10^-7
0
0
10
20
30
40
50
t
ES(t)


5. × 10^-7
4. × 10^-7
3. × 10^-7
P
2. × 10^-7
1. × 10^-7
0
0
10
20
30
40
50
t
P(t)




```
> display(plotS, plotE, plotES, plotP, plotEES, view = [0..50, 0..5·10^-7], labels = [t, ""])
```



Farver på den samlede graf:

GRØN = [S]
RØD = [P]
CYAN = [ES]
BLÅ = [E]
SORT = [E] + [ES]

NB: [E] + [ES] er konstant, dvs. enzymet forbruges ikke.
Substratet [S] forbruges, men produktet [P] fremstilles.